# IFPRI BRIEF TEMPLATE

**Check One:** ☐**Project** ☐**Review** ☐**Collaboration**
☐**Workshop** ☒**Other**

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| **Descriptive Title** | DEM Round Robin – Extension |
| **Working Title**[1] | DEM Round Robin II |
| **Technical Area**[2] | Characterization, Dry, Systems Engineering |
| **Date** | 06/21/2021 |
| **Short Description** | Extension of the current project for another term (2 years), providing further insight into the influence of particle shape, cohesion and the limitations of 'upscaling' particles to model smaller particles and/or larger systems. The extended project will also extend and test the generality of the best practices suggested in the initial project and explore a wider range of characterization tools so as to work toward establishing an optimal method for the characterization of particles' microscopic properties (friction, restitution, cohesion, etc.) and thus the calibration of DEM simulations. Finally, the extended project will provide a stronger emphasis on the modelling of stresses, including a systematic study on the effectiveness of different commonly-used force models. |
| **Objectives** | 1. Investigation of elongated/high aspect ratio particles<br>2. Investigation of fine powder (~100 um)<br>3. Investigation of stress field in the current systems<br>4. Once best practices of calibration are identified, investigate whether DEM can be used to inversely infer single particle and particle interactional properties<br>5. Including additional "DEM digital twins". Examples include:<br>o The new smaller Schulze Ring Shear Tester (RST.Xr)<br>o The Granutools GranuPack → tapped bulk density<br>o The Granutools GranuFlow<br>o Freeman Technology Uniaxial Powder Tester (UPT)<br>o The Anton Paar rheometer |
| **Scope** | 1. In the original Round Robin, it was determined that the dynamics of highly angular but relatively compact particles could be effectively and efficiently modelled using spherical particles with |

[1] Title used in meeting agendas and file archives
[2] One or more from the following list: W = wet systems; D = dry systems; F = particle formation; SR = size reduction; M = modeling; SE = systems engineering

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| | carefully calibrated rolling friction coefficients. Objective 1 aims to test the limitations of this model and, in the likely event of its breakdown at high aspect ratios, establish which alternative geometric model(s) are most effective, and how they are best calibrated. There exists scope also – if there exists an appetite within the membership – to explore the modelling of non-convex particles also.<br><br>2. In the original Round Robin, particles of sizes down to 300 micron were tested. In the extension, we propose to extend down to 100 micron. This will allow us to further explore the ability of DEM to simulate systems comprising large numbers of particles (thus better emulating the challenge faced in the modelling of 'real' industrial systems). In particular, it will allow deeper insight into the effectiveness of coarse graining schemes and their limitations. Materials suitable for PEPT imaging have already been selected.<br><br>3. The original Round Robin focused predominantly on the ability of DEM to reproduce the *dynamics* of industry-relevant systems but not the stress fields therein. In the extended project, a combination of in-line force measurements using a Lenterra force sensor and bulk torque measurements will be used to assess the ability of current DEM calibration methodologies and force models to correctly reproduce the stresses experienced by particles in dynamic systems.<br><br>4. In the first round of the round robin, Birmingham developed "digital twins" of a series of powder characterization tools which will be expanded in the 2nd term to the systems that IFPRI members are interested or commonly use. The digital twin simulations and the data extraction tools are all on open-source platforms and the team at **Birmingham has agreed to provide a series of training webinars on how to setup, run, and analyze the open-source digital twins during the 2nd term (similar to the arrangement we had for ADDICT software by Mike Doherty)**<br><br>5. In the original work, certain key elements of best practice for the calibration of DEM models were established, and more broadly the extraction of microscopic particle properties from bulk measurements. In the extended project, the additional time provided, combined with the additional digital twins to be developed as per objective 5, this best practice will be further developed, test the generality of our previous findings, and explore various additional manners in which one may rigorously and precisely frame and solve relevant 'inverse problems' to determine single particle and particle interactional properties from standard bulk measurements using widely-available characterization tools. |

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| | Team at Birmingham University are already exploring variety of methodologies, (e.g see https://slideslive.com/38945020/autonomous-characterisation-and-calibration-using-evolutionary-simulation-software)._ |

| Recommended Contractors (2 or 3) | | |
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